Pentanedioic acid, 3,3-dimethyl-4839-46-7 | DTXSID9063617

Model Performance

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N	Model	Data	

Weighted KNN model

5-fold CV (5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.87	0.81	0.87	0.82	0.86	0.86	

Model Results

Predicted value: 1.85e-01 mol/L

Global applicability domain: Inside

Local applicability domain index: 7.32e-01

Confidence level: 6.90e-01

Nearest Neighbors from the Training Set

Image not found

Heptanedioic acid Measured: 3.12e-01 Predicted: 1.47e-01

Image not found

2-propylbut-2-enedioic acid Measured: 7.02e-02 Predicted: 8.12e-02

Image not found

Octanedioic acid Measured: 6.79e-02 Predicted: 4.83e-02